

MASTER

TITLE GRADIENT SCALING FOR NONUNIFORM MESHES

LA-UR--85-1049

DE85 009625

AUTHOR(S) L. G. Margolin, LLNL (formerly in ESS-5)
H. M. Ruppel, T-3
R. B. Demuth, ESS-5

SUBMITTED TO: Fourth International Conference on
NUMERICAL METHODS IN LAMINAR AND TURBULENT FLOW
The University of Wales, Swansea, UK
July 9-12, 1985

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Los Alamos Los Alamos National Laboratory
Los Alamos, New Mexico 87545

GRADIENT SCALING FOR NONUNIFORM MESHES

L. G. Margolin
Lawrence Livermore National Laboratory
Livermore, California, 94550, U.S.A.

H. M. Ruppel and R. B. Demuth
Los Alamos National Laboratory
Los Alamos, New Mexico, 87545, U.S.A.

ABSTRACT

This paper is concerned with the effect of nonuniform meshes on the accuracy of finite-difference calculations of fluid flow. In particular, when a simple shock propagates through a nonuniform mesh, one may fail to model the jump conditions across the shock even when the equations are differenced in manifestly conservative fashion. We develop an approximate dispersion analysis of the numerical equations and identify the source of the mesh dependency with the form of the artificial viscosity. We then derive an algebraic correction to the numerical equations--a scaling factor for the pressure gradient--to essentially eliminate the mesh dependency. We present several calculations to illustrate our theory. We conclude with an alternate interpretation of our results.

1. INTRODUCTION

In finite difference methods, continuous solutions of systems of partial differential equations are represented by discrete values on a mesh. Although the solution to the differential equations themselves is clearly independent of the choice of mesh, the difference approximation depends on the details of the discretization and so varies with the choice of mesh. Nonetheless, if the problem is well-resolved, the numerical solution should closely approximate the true solution. As the mesh is refined, one requires that the numerical solutions converge to the true solution of the original system.

This is not always the case. Consider the simple one-dimensional problem of a piston-driven shock for which we specify the initial value of the thermodynamic variables (density, pressure, and internal energy), material velocity and the piston velocity. Then the shock speed, thermodynamic variables

and material velocity behind the shock are completely determined by the equation of state and the jump conditions [1], which express conservation of mass, momentum, and energy.

Kee, Kramer, and Noh [2] showed it is possible in a difference approximation to calculate the wrong values behind a shock even if the equations are differenced in a completely conservative fashion. The key features of their demonstration are the use of an initial mesh that is spatially nonuniform and an artificial viscosity that depends locally on the mesh scaling. Of even more concern is that the incorrect solution persists even as the mesh is refined, so long as the mesh remains nonuniform. Similar results have been reported by Lee and Whalen [3].

Other problems with nonuniform meshes are discussed by Kalnay de Rivas [4], Crowder and Dalton [5], Mastin [6], and Chin and Hedstrom [7]. Since it is not always possible to avoid using nonuniform meshes, and in fact there are significant advantages to variable resolution, it is essential to understand the source of these zeroth-order errors (errors that do not vanish as the mesh is refined and hence do not recover the differential equations) and to mitigate them.

In the past, truncation analysis has been the preferred method of investigating accuracy; however, dispersion analysis is an important tool in understanding the stability of difference equations [8]. More recently, Trefethsen [9] has pointed out the importance of group velocity in obtaining accurate calculations.

Margolin [10] looked at the simulation of stress waves in a viscoelastic solid. He performed an approximate dispersion analysis by considering the equivalent continuous equations and identified a spurious alteration of the sound speed due to coupling between artificial viscosity and the stress relaxation term. He then forced the numerical dispersion relation to approximate the physical relation by introducing a scaling factor into the stress gradient.

This technique, called gradient scaling, differs from simple subtraction of the truncation errors in at least two essential ways. First, it is not necessary to calculate any finite difference approximations to derivatives; the corrections are simply algebraic. Second, subtracting the truncation errors in the example above (of stress wave propagation) amounts to eliminating the artificial viscosity. Since this viscosity is necessary to damp numerical oscillations, its elimination is not a viable solution to the difficulty.

Both Trefethsen and Margolin dealt with regular meshes. To derive the dispersion relation, one substitutes the discrete approximation of a plane wave into the difference equations. The situation for nonuniform meshes is more complicated. Insertion of a plane wave into the difference equation leads to a relation in which frequency depends on the spatial coordinate

as well as on the wave number. This is analogous to wave propagation in an inhomogeneous medium. When the properties of the medium vary slowly, one can employ a two scale analysis [11].

With this introduction, we can now outline the rest of this paper. In the next section, we describe a simple problem of wave propagation on a nonuniform mesh. Calculations show a systematic error (when compared with analytic results) that does not decrease with mesh refinement. Next, we develop an approximate dispersion analysis to isolate the problem. The method of gradient scaling is then applied to the difference equations, and the new results are compared with both the uncorrected calculations and the analytic results. Finally, we discuss why strict conservation is not sufficient to guarantee the proper state behind a shock.

2. PROBLEM DESCRIPTION

We begin with the linearized equations for one-dimensional fluid flow, or for stress propagation in an elastic solid:

$$\rho \frac{du}{dt} = - \frac{\partial p}{\partial x} \quad (1)$$

$$\frac{dp}{dt} = -M \frac{\partial u}{\partial x} \quad (2)$$

Equation (1) expresses the conservation of momentum, where u is the material velocity and p is the pressure. Equation (2) is the constitutive law for the material. The density ρ and the modulus M are considered constant.

We solve a simple piston problem in which the pressure and material velocities are initially everywhere zero. In our model problem, the left boundary begins to move to the right at time zero, compressing the fluid, with Mach number of 0.2 and

$$u_{\text{left}} = 0.2 \sqrt{M/\rho} \quad (3)$$

We construct a staggered grid with pressures stored at cell centers and velocities at the nodes (see Fig. 1).

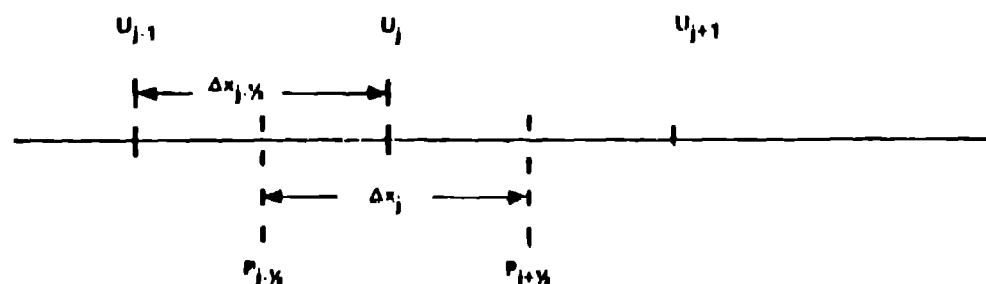


Fig. 1. Configuration of the staggered grid.

Our difference equations are

$$\frac{p_{j+\frac{1}{2}}^{n+1} - p_{j+\frac{1}{2}}^n}{\Delta t} = -M \frac{u_{j+1}^n - u_j^n}{\Delta x_{j+\frac{1}{2}}} \quad (4)$$

$$\begin{aligned} \rho \frac{u_j^{n+1} - u_j^n}{\Delta t} = & - \frac{p_{j+\frac{1}{2}}^{n+1} - p_{j-\frac{1}{2}}^{n+1}}{\Delta x_j} \\ & + \frac{1}{\Delta x_j} \left(\frac{\lambda_{j+\frac{1}{2}} (u_{j+1}^n - u_j^n)}{\Delta x_{j+\frac{1}{2}}} - \frac{\lambda_{j-\frac{1}{2}} (u_j^n - u_{j-1}^n)}{\Delta x_{j-\frac{1}{2}}} \right). \end{aligned} \quad (5)$$

Here the superscript n refers to time level $t^n = n\Delta t$, where Δt is the time step. The time step must be limited by a Courant condition for stability [8].

We have introduced an artificial viscous pressure into Eq. (5) to suppress numerical oscillations [12]. The coefficient λ is chosen to have the form

$$\lambda_{j+\frac{1}{2}} = c_L \sqrt{\rho M} \Delta x_{j+\frac{1}{2}}. \quad (6)$$

We have made the length scale equal to the local cell size, so that the wave front is spread out over a fixed number of cells rather than a fixed length. In our numerical example we choose the dimensionless coefficient $c_L = 0.2$, which results in the wave being spread over about three cells.

We pick a constant ratio for the mesh spacing

$$\alpha = \frac{\Delta x_{j+\frac{1}{2}}}{\Delta x_{j-\frac{1}{2}}}. \quad (7)$$

If α equals 1, we have a uniform mesh. If α is greater than 1, the mesh is expanding; if α is less than 1 the mesh is contracting. The width of the first cell is

$$\Delta x \equiv \Delta x_{3/2}. \quad (8)$$

The results for several choices of α are shown in Figures 2, 3, and 4. The uniform case ($\alpha = 1$) yields the correct solution. However, when $\alpha > 1$ we see that the pressure behind the front is too high; when $\alpha < 1$, the pressure is too low. Moreover, the speed of the front is too slow when $\alpha > 1$ and too fast when $\alpha < 1$. We note that in each case, the pressure behind the front does reach a level value. Note that the amount of overshoot or undershoot is approximately linear in $(\alpha - 1)$.

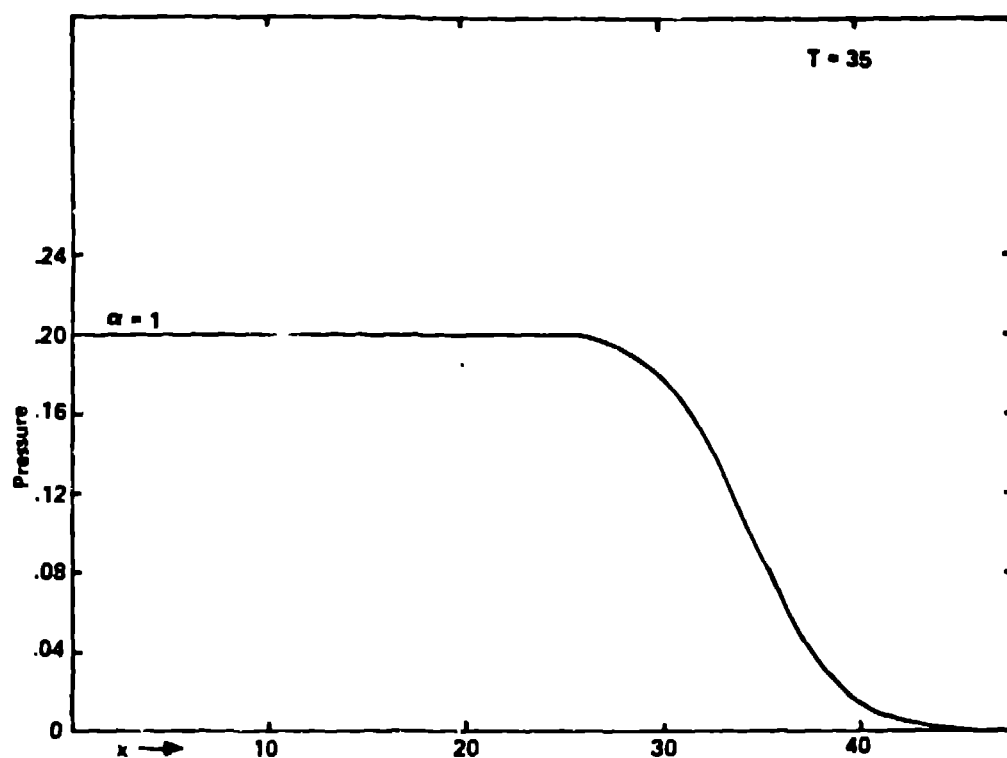


Fig. 2. Pressure profile for piston driven shock on a regular grid.

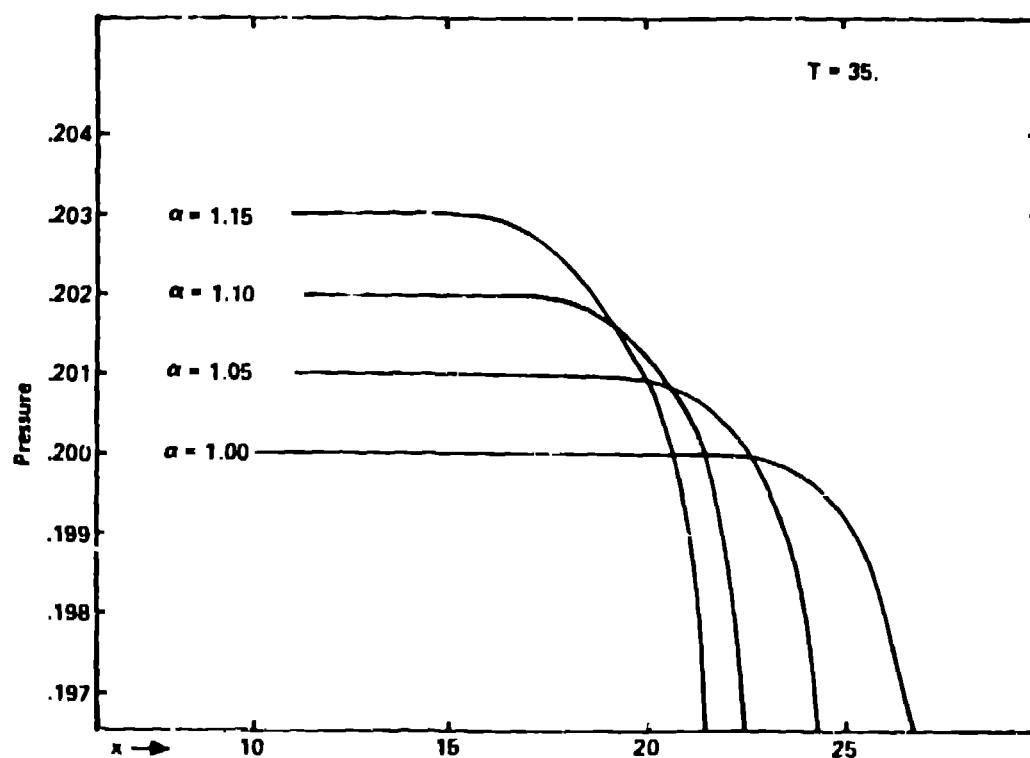


Fig. 3. Pressure profiles on a mesh with increasing grid spacing for several values of α . Note that Fig. 3 is a window of Fig. 2 with a scale change to show the effect.

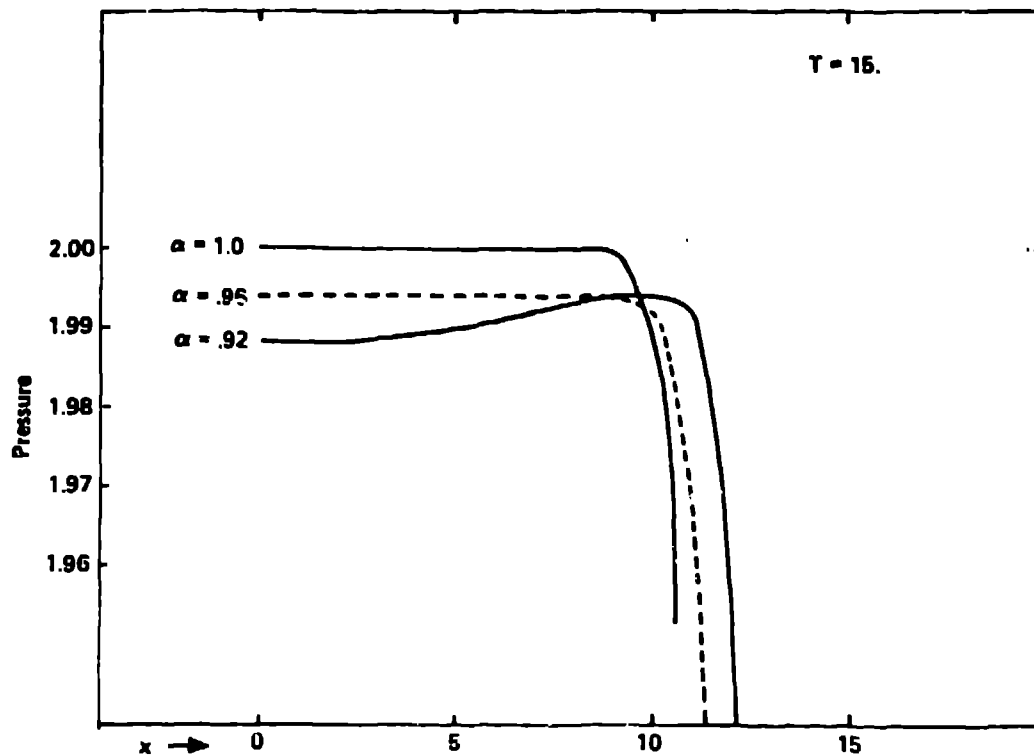


Fig. 4. Pressure profiles on a contracting grid. Note time scale change compared to Figs. 2 and 3.

To perform the dispersion analysis on a uniform mesh, we would substitute

$$u_j^n = u_0 \exp i(kx - \omega t) \quad (9)$$

and so generate the dispersion relation. However, if $\alpha \neq 1$, then in our Eqs. (4) and (5) this substitution results in a relation between wave number and frequency that involves the mesh size. This seems to imply that the wave speed has become dependent on position. However, the numerical simulations indicate that the wave speed, while incorrect if $\alpha \neq 1$, nevertheless is constant for the constant ratio meshes. In the next section, we will describe an approximate dispersion analysis that resolves this situation.

3. APPROXIMATE DISPERSION ANALYSIS

Our analysis can be summarized as follows. First, we will expand the difference equations using Taylor series to derive a set of equivalent continuum equations. Then we will find approximate solutions in the form of plane waves with small perturbations. Finally, we will reinterpret these perturbations as alterations of the effective wave number.

Expanding the difference Eqs. (4) and (5), we derive the equivalent continuum equations

$$\rho \frac{du}{dt} = - \frac{\partial p}{\partial x} + A \frac{\partial u}{\partial x} + (Ax + B) \frac{\partial^2 u}{\partial x^2} \quad (10)$$

and

$$\frac{dp}{dt} = -M \frac{\partial u}{\partial x} \quad (11)$$

(We have used the relation

$$x_j = \Delta x (1 + \alpha + \dots \alpha^{j-2}) \quad (12)$$

in deriving Eq. (10).)

The constants in Eq. (10) are given by

$$A = 2 c_L \sqrt{\rho M} \left(\frac{\alpha - 1}{\alpha + 1} \right) \quad (13)$$

$$B = c_L \sqrt{\rho M} \left(\frac{\alpha - 1}{\alpha} \right) \Delta x \quad .$$

The expansion has been truncated by including terms only to first order in the small quantity $(\alpha - 1)$.

From Eqs. (10) and (11), we can form the wave equation for the velocity

$$\rho \frac{d^2 u}{dt^2} = M \frac{\partial^2 u}{\partial x^2} + A \frac{\partial^2 u}{\partial x \partial t} + (Ax + B) \frac{\partial^3 u}{\partial x^2 \partial t} \quad (14)$$

We seek solutions to this equation as slight perturbations of plane waves. In particular, we try

$$u = u_0 (1 + ax + bx^2) \exp i(kx - \omega t) \quad , \quad (15)$$

which leads to

$$k^2 M = \rho \omega^2 \quad (16)$$

for the physical dispersion relation.

Substituting Eq. (15) into the wave equation Eq. (14), we find, to first order in $(\alpha - 1)$ and also in $k\Delta x$,

$$a = \pm \frac{1}{2} c_L \left(\frac{\alpha - 1}{\alpha + 1} \right) k \quad (17)$$

$$b = \pm \frac{1}{2} c_L \left(\frac{\alpha - 1}{\alpha + 1} \right) k^2 \quad .$$

Now in a region near the origin (i.e., $x \approx 0$), we have

$$(1 + ax) \sim \exp(ax) \quad (18)$$

Making use of this approximation we can rewrite Eq. (15):

$$u = u_0 \exp (i(k'x - \omega t)) \quad , \quad (19)$$

where k' is an effective wave number. Using Eq. (17), we find that

$$k' = k \left(1 \pm \frac{c_L}{2} \left(\frac{\alpha - 1}{\alpha + 1} \right) \right) \quad . \quad (20)$$

Here the $(-)$ sign refers to waves traveling to the left and the $(+)$ sign to waves traveling to the right.

In our analysis α is constant over the mesh; there is nothing special about the origin except that it specifies our choice of Δx . As long as $k\Delta x \ll 1$, we could expand about any point with a similar result. That is, the effective wave number k' , and the associated phase and group velocities

$$c' = \frac{\omega}{k'} = \frac{d\omega}{dk'} = \frac{\sqrt{M/\rho}}{\left[1 \pm \frac{c_L}{2} \left(\frac{\alpha - 1}{\alpha + 1} \right) \right]} \quad (21)$$

are constant over the mesh. (To the order to which we are interested in this analysis, the phase and group velocities are equal to each other, as they are in our physical example.) This verifies the existence of a flat pressure profile behind the shock. Note the fundamental asymmetry between left- and right-going waves because of the asymmetry in zoning. The wave moves too fast if it moves into a region of expanding zones.

If α varies over the mesh, then the effective wave number will also vary. However, as long as this variation is slow, our analysis will hold locally. Of course, if α varies rapidly, then our derivation of Eq. (14) is not valid. The form of the effective phase and group velocities verifies our numerical experiments in that the error is approximately linear in $(\alpha - 1)$. It also illustrates that the error, to lowest order, is independent of Δx , and so will not vanish as the mesh is refined.

4. GRADIENT SCALING

To mitigate the effects of nonuniform zoning, we introduce a scaling factor, β , for the pressure gradient into the difference Eq. (5). This is, now

$$\rho \frac{u_j^{n+1} - u_j^n}{\Delta t} = -\beta \frac{p_{j+1}^{n+1} - p_{j-1}^{n+1}}{\Delta x_j} + \dots \quad (22)$$

Expanding our new set of difference equations as before, and then forming a wave equation for velocity, we derive

$$\rho \frac{d^2 u}{dt^2} = \beta M \frac{\partial^2 u}{\partial x^2} + A \frac{\partial^2 u}{\partial x \partial t} + (Ax + B) \frac{\partial^3 u}{\partial x^2 \partial t} \quad . \quad (23)$$

Again, we try as a solution the form of Eq. (15)

$$u = u_0(1 + ax + bx^2) \exp [i(kx - \omega t)] .$$

Now, however, we ask whether we can choose β so that $a = 0$.

In fact, this can be accomplished if we choose

$$\beta = 1 \pm c_L \left(\frac{\alpha - 1}{\alpha + 1} \right) , \quad (24)$$

where the plus sign applies to right-going waves.

When the gradient scaling term is used in our prototypical piston problem, the results are clearly improved. For each choice of α , Table I shows that the error is reduced by about an order of magnitude. This is consistent with our analysis, which ignored terms of order $(\alpha - 1)^2$.

α	Pressure	
	uncorrected	corrected
1.00	.20000	--
1.05	.20103	.20000
1.10	.20201	.20001
1.15	.20302	.20021
1.00	.20006	--
.96	.19941	.20002
.92	.19883	.20008

Table I. Comparison of the level values of pressure behind the shock. The last column shows the results of a calculation with gradient scaling. The results of the expanding mesh used a different viscosity than those of the contracting mesh, and so are not directly comparable.

In our final example, we consider a nonuniform mesh with a variable value of α . The zoning has a sinusoidal variation

$$\Delta x_j = 1 + .2 \times \sin \left(\frac{2\pi}{10} j \right) \quad (25)$$

The zoning has a wavelength of ten cells, so α is greater than 1 for 5 cells and is less than 1 for the next 5 cells.

The results of a calculation on this mesh are shown in Fig. 5. The pressure amplitude shows a similar sinusoidal variation, slightly lagging the zonal variation in phase. The uncorrected calculation has a maximum excursion comparable to a calculation using a constant value of $\alpha = 1.07$. Using the pressure gradient scaling we realize a reduction of error by about a factor of five. Since α is not a constant in this example, β must be evaluated locally. We determined $\beta_{j+\frac{1}{2}}(\alpha)$ from Eq. (24) with $\alpha_{j+\frac{1}{2}} = \Delta x_{j+1} / \Delta x_j$.

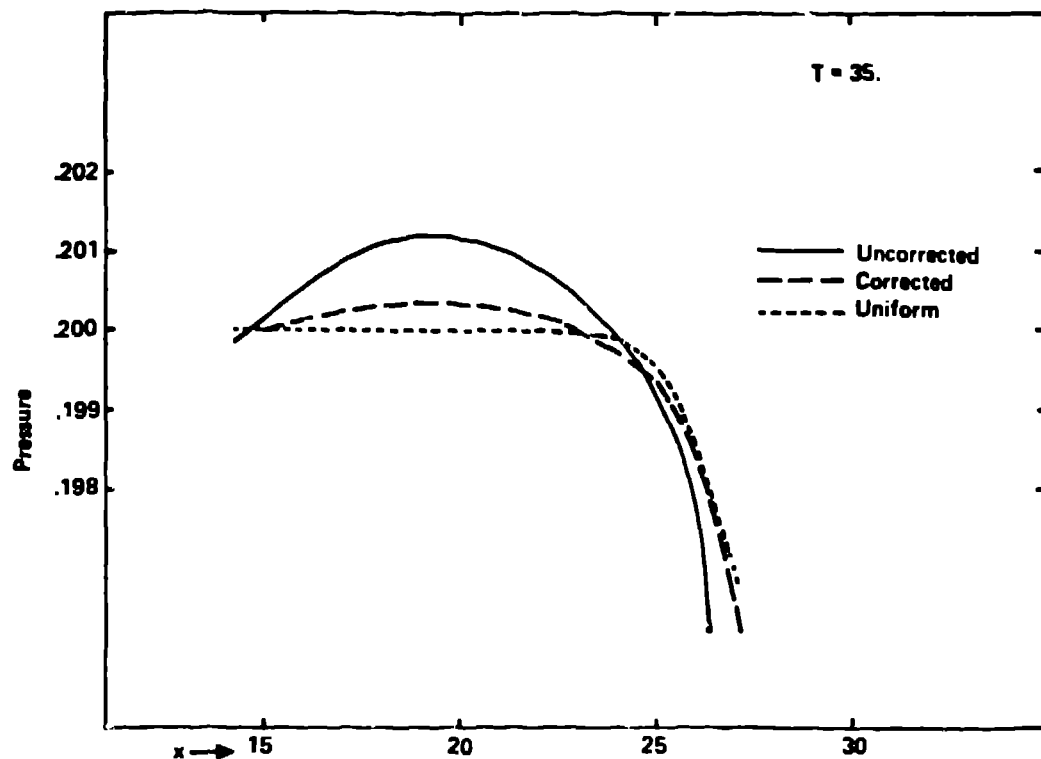


Fig. 5. Pressure profile for a sinusoidally varying grid spacing. The constant spacing solution is included for comparison.

5. DISCUSSION

We conclude by reinterpreting our results in terms of the jump conditions. In the following paragraphs, we use the term "shock" to mean the transition between some uniform initial state and some other uniform final state.

Physically, the thermodynamic jumps across a shock and the shock speed are uniquely determined by the equations of conservation of mass, momentum and energy, plus the equation of state. (An entropy principle to guarantee a flat profile is also required.) On a uniform mesh, conservative differencing will allow one to calculate the precise jumps. As we have seen, on a nonuniform mesh, this is no longer true.

The explanation lies in the form of the artificial viscosity, which spreads the shock over a fixed number of cells rather than over a fixed length. As the shock propagates, its width is steadily changing. Thus, the mass swept up by the shock is not the mass coming out the back end. In essence, the shock transition is acting as a source or sink of mass, as well as the associated momentum and energy.

The dispersion of the shock front does not depend on wave number, but rather on the coordinate. It is due to the term

$$Ax \frac{\partial^3 u}{\partial x^2 \partial t}$$

in the wave equation Eq. (14). Associated with this dispersion, the shock moves with a slightly incorrect velocity [Eq. (19)]. If we approach this problem with truncation analysis, we would identify the terms in the equivalent continuum Eqs. (10) and (11) that have coefficient A. Our solution would be to estimate these terms numerically and subtract them out. This is equivalent to using only a "fixed length" viscosity.

The difficulty with this approach is the technique to choose this fixed length. The role of the artificial viscosity is to prevent numerical oscillations behind the shock. To accomplish this, the length scale embedded in the viscous coefficient must be comparable to the size of a cell. (For a more detailed discussion of artificial viscosity, see Wilkins [14].) If the fixed length is chosen as large as the biggest cell, we will have excess smoothing in a region of smaller cells. If the fixed length is chosen any smaller, than we will develop oscillations in the region of large cells.

Our solution, based on dispersion analysis, does not affect the dispersion of the shock front. It does change the effective wave speed. In terms of the jump conditions, once we have specified the conservation of mass, momentum and energy, the only freedom we have remaining is the equation of state. Indeed, the gradient scaling factor has the effect of altering the compressibility of the fluid. This new compressibility ensures that the amount of mass and momentum coming out the back end of the shock is appropriate to yield the proper jumps in these variables.

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